Mandelic acid

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 7.54e-01

Global applicability domain: Inside

Local applicability domain index: 6.34e-01

Confidence level: 8.91e-01

Nearest Neighbors from the Training Set

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Mandelic acid
Measured: 0.62
Predicted: 7.54e-01

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Salicyl alcohol
Measured: 0.73
Predicted: 7.49e-01

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3-Hydroxybenzyl alcohol
Measured: 0.49
Predicted: 6.45e-01